TOPAZ/TOPAZCHM Modeling Codes

Allows modeling a wide range of problems

At LLNL, we have developed a suite of codes that have been used successfully to model a wide range of problems. Chief among these codes are DYNA2D and DYNA3D (explicit finite-element codes), NIKE2D and NIKE3D (implicit finite-element codes), and TOPAZ2D (implicit heat-transport code). The heat-flow code TOPAZ2D has been modified to incorporate arbitrary chemistry of mixed materials with Arrhenius kinetics.

TOPAZCHM for modeling chemical reactions

This new code has all of the thermal capabilities of the original TOPAZ code:

- Several boundary conditions:
  - Temperature
  - Flux
  - Convection
  - Radiation
  - Enclosure radiation.
- Thermal slidelines.
- Internal heat generation.
- Bulk nodes.
- Nonisotropic thermal conductivity.

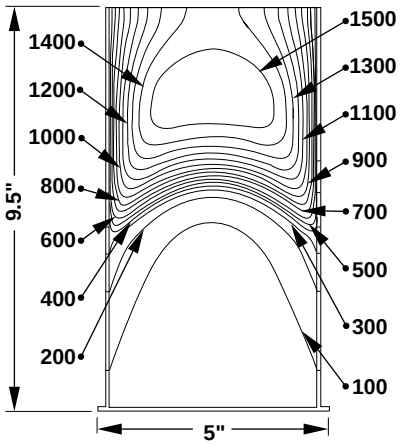
In addition, TOPAZCHM has the capabilities needed to handle chemical reactions:

- Improved time-step control.
- Several mixture models for thermal conductivity and heat capacity.
- Gas production.
- Arrhenius kinetics with activation volume and pressure prefactor terms.

APPLICATIONS

- *Modeling the response of explosives to fire*
- *Modeling thermite reactions*
- *Modeling phase transitions in solids*
- *Modeling hazards in a fire*

TOPAZCHM currently is being used successfully to model several widely different systems. Although the underlying theory is straightforward, we have been able to develop several phenomenological chemical reaction models that can be applied to a range of problems. For example, models have been constructed to study thermochemical processes such as thermite burns; the time-to-event for a heated, confined explosive; the deflagration of nonconfined explosives; and complex phase transitions. This same methodology can be applied to diverse problems such as rain flow and curing in injection molding.



Temperature profiles in a cylinder of burning explosive (LX17) 20 minutes after ignition.

PALM2D for modeling simultaneous heat and stress

This code adds to TOPAZ2D all of the capabilities of NIKE2D:

- Many elastic and inelastic material models.
- Several types of slidelines.
- Several boundary conditions:
  - Pressure
  - Shear
  - Displacement.
- Thermal stress.
- Body loads.
- Nodal loads.

PALM2D has been used to model problems with simultaneous heat and stress loads. The TOPAZCHM and PALM2D codes can be used together to solve coupled thermal–mechanical–chemical problems.

Availability: These codes are available now; LLNL is seeking industrial partners with whom to apply the codes to industry needs.

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